1,4-Dioxane
123-91-1 | DTXSID4020533

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 7.30e-12 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.20e-01

Confidence level: 7.56e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
1,4-Dioxane	2-Chloroethanol	2-Methyl-1,3-dioxolane
Measured: 1.09e-11	**Measured:** 1.40e-12	**Measured:** 9.40e-12
Predicted: 7.30e-12	**Predicted:** 2.40e-12	**Predicted:** 9.84e-12

Image not found	Image not found
Ethane, 1-bromo-2-methoxy-	Ethane, 1-chloro-2-methoxy-
Measured: 6.64e-12	**Measured:** 4.69e-12
Predicted: 8.17e-12	**Predicted:** 4.24e-12